Acifluorfen, heptyl ester

Inchi: InChI=1S/C21H21ClF3NO5/c1-2-3-4-5-6-11-30-20(27)16-13-15(8-9-18(16)26(28)29)31-1
InchiKey: MQXAHNZQJKOPBR-UHFFFAOYSA-N
Formula: C21H21ClF3NO5
SMILES: CCCCCCCOC(=O)c1cc(Oc2ccc(C(F)(F)F)cc2Cl)ccc1[N+](=O)[O-]
Mol. weight [g/mol]: 459.84

Physical Properties

Property code	Value	Unit	Source
gf	-584.65	kJ/mol	Joback Method
hf	-1050.19	kJ/mol	Joback Method
hfus	58.03	kJ/mol	Joback Method
hvap	98.33	kJ/mol	Joback Method
log10ws	-8.30		Crippen Method
logp	7.187		Crippen Method
mcvol	307.510	ml/mol	McGowan Method
pc	1328.10	kPa	Joback Method
rinpol	3107.00		NIST Webbook
rinpol	3107.00		NIST Webbook
tb	1035.72	K	Joback Method
tc	1272.59	K	Joback Method
tf	701.46	K	Joback Method
vc	1.212	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	966.87	J/mol×K	1035.72	Joback Method
cpg	976.89	J/mol×K	1075.20	Joback Method
cpg	985.71	J/mol×K	1114.68	Joback Method
cpg	993.41	J/mol×K	1154.15	Joback Method
cpg	1000.05	J/mol×K	1193.63	Joback Method
cpg	1005.72	J/mol×K	1233.11	Joback Method
cpg	1010.47	J/mol×K	1272.59	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415146&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume